International Journal of Physics
And Research (IJPR)
ISSN(P): 2250-0030; ISSN(E): 2319-4499
Vol. 6, Issue 4, Aug 2016, 11-16

TRANS STELLAR
•Journal Publications •Research Consultancy

ELECTRONIC AND THERMODYNAMIC PROPERTIES OF NAOH

DUKRA KAMAL TAHA

Ministry of Education Academic, Baghdad, Iraq

ABSTRACT

The study of spectral of multi molecules by theoretical and experimental, theoretical parts, Where the theoretical part using Gaussian 09 program which include study of the NaOH molecules using DFT methods, but experimental part which studies by tacking solution of the spectropics behavior of molecules gives all parametrizes to known Nature of this molecules from calculation energy gaps. In addition to calculation all of heat capacity ($C_{0p,m}$), entropy (S_{0m}) and enthalpy (H_{0m}).The Density functional ways used B3LYP / [6-311 G**, aug-cc-pVQZ, SDD] bases sets as well as its good agreements with experimental parts.

KEYWORDS: NaOH, DFT methods, Theoretical Parts

Received: Jun 21, 2016; **Accepted:** Jul 08, 2016; **Published:** Jul 16, 2016; **Paper Id.:** IJPRAUG20162

Original Article

INTRODUCTION

Sodium hydroxide consideration as an inorganic compound. Seems as white solid and highly caustic metallic base and alkali salt which is available in pellets, flakes, granules, and as prepared solutions at a number of different concentrations. [1]

While thermodynamics mathematical system for describing energy and entropy in macroscopic chemical systems entropy is the driving force for causing the randomly chains. While thermodynamics mathematical system for describing energy and entropy in macroscopic chemical systems [2,3].

EXPERMANTAL

MATERIALS

Sodium hydroxide contains of three molecules hydrogen, oxygen and nitrogen the structures showed in figure 1.

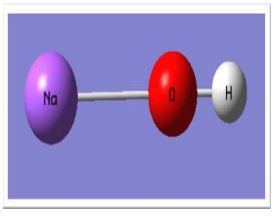

Figure 1: The NaOH Molecule

PREPARED METHODS

The solution prepared throught soluble Sodium hydroxide in pure Dioxins 99.99 % to produce concentrations $1x10^{-3}$ M. Then using ShimadzuUV-3101PCUV-VIS-NIR spectrophotometer. [5]

THEORETICAL WORKS

This works gives indicators divided into about optimizations of the molecules, the highest points on the conductors bands and lowest points into the valance bands to extraction energy gaps values. In addition to zero potential energy for NaOH molecules

RESULTS

The absorption peaks shows in figure 2

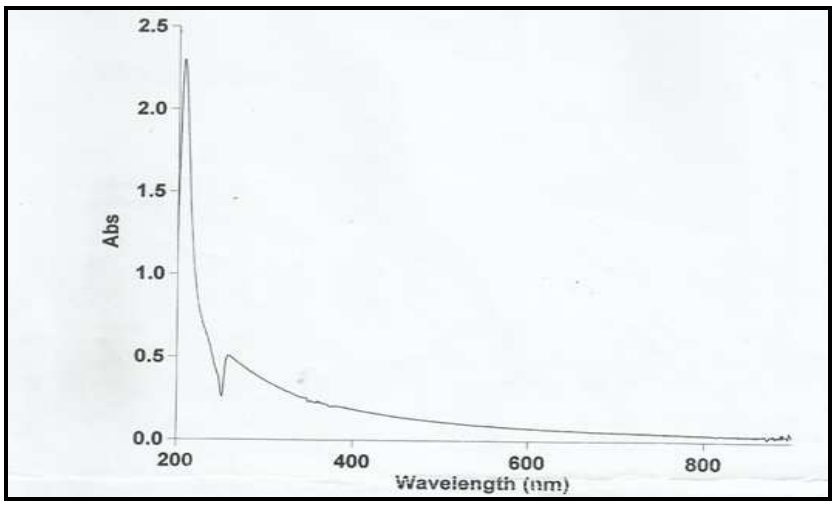

Figure 2: The Absorption Spectrum

The NaOH fluorescence shown in figure 3

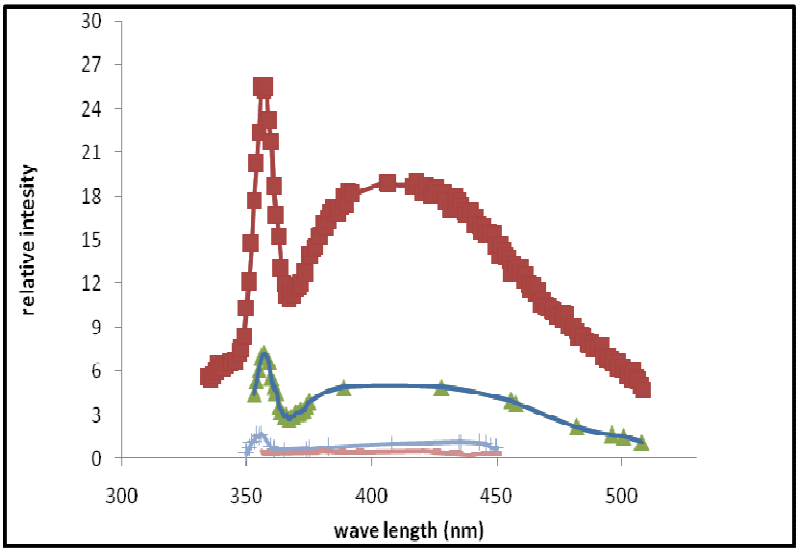

Figure 3: The Fluorescence of NaOH

The different concentration of solutions leads to high wave length shifted results from many no radiation transmissions as shown in table 1

Table 1: Shows the Fluorescence Peaks and Band Width

Width	Relative Intensity (a.u.)	λ_{max}flu(nm)	Band Width $\Delta\lambda$ (nm)
13spc	0.506	421	44.379
53spc	1.65	365	352.36
55spc	7.176	357	353.26
33spc	25.64	356	352.37

THEORETICAL RESULTS

Three bases sets of the Density function theory which using for studying electronic and thermodynamics properties for NaOH molecules.

Density functional theory considerable as accuracy methods to produce structure optimization and total energies.

The structure of Sodium Hydroxide gated through using B3LYP / [6-311 G**] the results for these molecules as shown in table 2.

Table 2: Shows the Structure NaOH

Parameters	6-311G**
Na1 – O2	1.90523
O2 – H3	0.95878
Na1 – H3	2.8032
∠Na1O2H3	180.0001

THE ENERGY GAP

Results showed that's good agreement with previous studies as if it decreasing id each height and lowest states in negative values this seen that's a stable molecules as shown in table 3

Table 3: Shows Results of Height and Lowest States

	DFT	Homo	Lomo	E_g theoretical results	E_g experimental results
Density function theory	B3LYP/6-311G*	-4.6300	-1.6150	3.0150	3.05
	B3LYP/6-311G**	-4.6170	-1.6063	3.0107	3.05
	B3LYP/6-31G(2df,p)	-4.7424	-1.4229	3.3195	3.05
	B3LYP/aug-cc-pVQZ	-5.0363	-1.6158	3.4205	3.05
	B3LYP/SDD	-4.5204	-1.6076	2.9127	3.05

THE PHYSICAL PROPERTIES

The ionize potential IP, electron affinity EA, electro negativity χ, chemical hardness Ŋ, softness S and electrophonic index ω consideration as important physics characteristics, so results showed in table 4

Table 4: Physical Characteristics

Physical properties	Density functional theory / B3LYP		
	6-311G**	aug-cc-pVQZ	SDD
IP	4.617	5.0363	4.5204
EA	1.6063	1.6158	1.6076
κ	3.11165	3.32605	3.064
η	1.50535	1.71025	1.4564
S	0.332149	0.292355	0.343312
ω	3.215985	3.234208	3.223049

The thermodynamic extracted by Density functional / method results are shown in Table 5 and 6. The heat capacities, entropies and enthalpies were obtained by using B3LYP/6-311G **. According to the results, the increase of temperature increases heat capacities, entropies and enthalpies due to increasing intensities of molecular vibration. The correlation equations between heat capacities, entropies, enthalpies and temperature are shown below and can be used for analyzing heat capacities, entropies and enthalpies at different temperatures [9, 10]

Table 5: Thermodynamics Properties B3LYP/6-311G

Contribution	Entropy (J K^{-1} mol^{-1})	Integrated Heat Capacity (kJ mol^{-1})	Heat Capacity (J K^{-1} mol^{-1})
Translation	153.75	5.997	19.97
Rotational	68.18	3.834	12.88
Vibrational	32.68	2.842	12.99
Electronic	0.00	0	0
Total	254.61	12.673	45.84

Table 6: Thermodynamics Properties B3LYP/Aug-Cc-Pvqz

Contribution	Entropy (J K^{-1} mol^{-1})	Integrated Heat Capacity (kJ mol^{-1})	Heat Capacity (J K^{-1} mol^{-1})
Translation	153.12	6.972	19.98
Rotational	60.22	2.079	8.31
Vibrational	23.79	3.987	20.75
Electronic	0	0	0
Total	237.13	13.038	49.04

CONCLUSIONS

Using Gaussian 09 program to gets theoretical results of sodium hydroxide gives a good approximate method that developed and gets Gives the semi as a result practical results. The results obtained by the calculation for thermodynamics properties showed Favorable results with practical results

REFERENCES

1. *M.Safarikova, "European Cells and Materials", Vol 3, Suppl. 2, ISSN 473-2262, p188-191, (2002).*
2. *K.Okudaira, H.Setpyama, Journal of Electron Spectroscopy, N 263-8522, p 137-140, (2004).*
3. *Jeyakodi Moses J. and Pitchai S.: A Study on the Dyeing of Sodium Hydroxide Treated Polyester / Cotton Blend Fabrics, International Journal of Science, Technology and Society; 3(1-1): 1-9, (2015)*
4. *Mustafa Arık, Neslihan C¸ elebi, Yavuz Onganer, Fluorescence quenching of fluorescein with molecular oxygen in solution,*
5. *Journal of Photochemistry and Photobiology A: Chemistry 170 105, (2005).*
6. *Robert Sjoback, Jan Nygren, Milkael Kubista, Absorption and Floure scencce, Spectrochimica Acta Part A, 51, 17-21, (1995).*
7. *Andreas,Stadler (2012). Transparent Conducting Oxides-An Up-to-Date Overview,Materials, 5, 661-683.*
8. *F. Yakuphanoglu, S.Ilican, M. Caglar, Y. Caglar, Superlattices and Microstructures 47 (2010) 732_743.*
9. *Ç. Albayraka,, B. Kosara, M. Odabasoglub and O. Buyukgungor, J. Iran. Chem. Soc., Vol. 8, No. 3, September 2011, pp. 674-686.*
10. *David C. Young, COMPUTATIONAL CHEMISTRY, A JOHN WILEY & SONS, INC., PUBLICATION New York, 2001*